

# THE NUCLEUS

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## Monthly Meeting

*Julius F. Remenar, Alkermes, to speak on "Getting the most from salts and Co-crystals: formulating to maximize oral absorption"*

## Summer Scholar Report

*By Patrick Kelleher, Cameron Hill, Yongli Huang, Nan Chen, Deno del Sesto, Arthur Utz*

## International-Domestic Student Summit

*By Justin Foy with photos by Morton Z. Hoffman*

## January Meeting Report

*By Michael P. Filosa, photos by Morton Z. Hoffman*

# Reflecting on the International-Domestic Student Summit

By Justin Foy (Photos by Morton Z. Hoffman)

Department of Chemistry, Dartmouth College, 6128 Burke Hall, Hanover, NH 03755



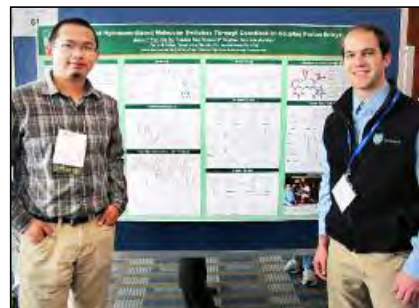
Xin Su (at left) with Morton Hoffman (Boston University) and Justin Foy

The International-Domestic Student Summit (IDSS) was held in Raleigh, NC with nine teams of two students each (one international and one domestic) from universities in the following local sections: Ames, Central New Mexico, Coastal Georgia, Colorado, Dallas-Fort Worth, East Central Illi-

nois, Kansas State University, New York and Northeastern. The purpose was for the ACS to get feedback from these students on how to promote international and domestic student collaboration, increase international skill flow, and utilize the unique resources that the international community provides. A study related to this overarching problem found that 38% of foreign students studying in the U.S. did not have a single close American friend.<sup>1</sup> As the largest scientific network, the ACS was determined to figure out what it was or wasn't doing well in serving of the international student.

I am the domestic student on this side of the equation. I was raised in Concord, NH and have never really moved far from home. The cross-cultural friendship statistic surprised me very much, as did the responses I received when I mentioned it. For

example, one international student in my department simply said in an apathetic tone "it can happen." Sure I was aware that there were cultural barriers before, but to see such a staggering number and to hear such an attitude about the subject was very strange. I started realizing that this is a much larger problem than I had previously thought.



Graduate students Xin Su (at left) and Justin Foy at their research poster, "Activation of Hydrazone-Based Molecular Switches Through Coordination Coupled Proton Transfer"

My partner to the conference was my labmate and friend Xin Su who is from Qinhuangdao, China. Xin and I set out on a brisk November morning from the Lebanon, NH airport. We were lucky to have perfect weather that day as we flew out in a small Cessna plane to Boston and subsequently down south to Raleigh. We had our first meeting that night at dinner with all of the other teams. This was our first introduction to Steve Meyers from the ACS who had coordinated the event. It was exciting to meet everyone for the first time and to see that we had a very diverse group where a good dialogue on international collaboration could be formulated.

During the IDSS summit, the participants were split into three different groups to analyze the problem from the perspective of local institutions, the ACS, or the global scientific commu-

*continued on page 4*

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**Cover:** A photo from the January Meeting held at the Heibert Lounge at Boston University School of Medicine. (L-R) Liming Shao, 2013 NESACS Chair; Ruth Tanner, 2012 NESACS Chair; Dr. Allen C. Steere, Harvard Medical School, and Catherine E. Costello, 2013 NESACS Chair-Elect. Photo by Morton Z. Hoffman

**Editorial Deadlines:** May 2013 Issue: March 15, 2013  
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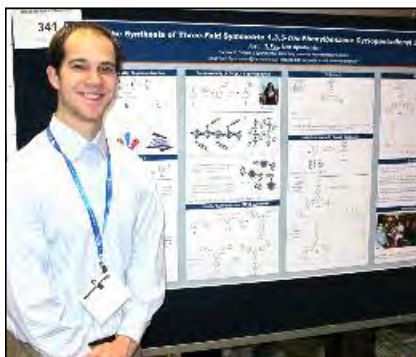
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## Student Summit

continued from page 2

nity. I was assigned to the global scientific community group and we tried to break down the global network into its respective institutions such as the funding agencies, special interest groups, universities, government, among many others. We began to see that many of these stakeholders in the global network that benefit from international researchers and collaborators are poorly coordinated with one another. One of the major suggestions was that the ACS could reach out to these groups and act as the “glue” with which to build a database of information to share between the stakeholders. We believe that increasing the networking ability between communities should also help get more opportunities for international students, whether it is in the form of discussion groups at a university or getting more out of the embassies.

There were many layers to the discussions that went on during the day. The most interesting part of the discussions for me was hearing the stories



Justin Foy at his research poster, “The Synthesis of Three-Fold Symmetric 1,3,5-tris-Phenylbenzene Cyclopentadienyl Ligands”

from the international students. Some told sad stories of not being able to get home for a death in the family because of visa difficulties, or some clearly were set behind in their careers because of the lack of opportunities in their home country. It certainly made me feel lucky to be born in a country with such a wealth of opportunity and, furthermore, that there are organizations in this country like the ACS that are trying to make a difference for everyone. At the end of the day, all of the groups were called together to summarize their suggestions.

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A recurring theme from all of the groups was the aim to increase the networking and sharing of information through social media. One area where this could be useful would be a blog containing societal logistics for a city/state/university (e.g. licensing, banks, shopping etc.). Another useful idea was to utilize a network of expatriates from each region to help mentor incoming students and prepare them better for the culture here. It was clear that an increasing amount of attention should be given at universities to hold partnering/mentoring events between international and domestic students to make them feel more welcome in this country. An exhaustive report of what was discussed is not possible here, but will be forthcoming from the ACS.

Everyone at the summit realized that the common obstacles that divide us, such as fundamental language/cultural barriers and visa problems, would not be changed overnight. Nonetheless,

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# Monthly Meeting

*The 931<sup>st</sup> Meeting of the Northeastern Section of the American Chemical Society*

**Thursday, March 14, 2013**

**MIT Faculty Club,**

50 Memorial Drive, Cambridge, MA 02142

**4:30 pm Board Meeting**

**5:30 pm Social Hour**

**6:30 pm Dinner**

**7:30 pm Welcome**

Dr. Liming Shao, Chair, NESACS

**Speaker**

Dr. Julius F. Remenar, Research Fellow, Alkermes, Waltham, MA.

**Title:** *Getting the most from salts and Co-crystals: formulating to maximize oral absorption*

Dinner Reservations should be made no later than 12:00 noon, Thursday, March 7th. Reservations are to be made using PayPal services: <http://acssymposium.com/paypal.html>. Select pay with credit or debit card option and follow the additional instructions on the page. Members, \$30; Non-members, \$35; Retirees, \$20; Students, \$10, Unemployed \$10. Reservations for new members only. For additional information contact the secretary, Anna Singer, between 9 am and 6 pm at (phone/fax 781-272-1966) or [secretary@nesacs.org](mailto:secretary@nesacs.org). Reservations not canceled at least 24 hours in advance must be paid.

THE PUBLIC IS INVITED

# Biography

Jules Remenar is a Research Fellow at Alkermes in Waltham, MA where his work is focused on understanding the physical behavior of drug molecules as they interact with formulation components during manufacture, on storage, and after dosing.

Dr. Remenar received a Bachelors degree in chemistry from Michigan State University in 1991 and a Ph.D. in physical-organic chemistry from Cornell University in 1996. He completed studies in polymers and materials science as a postdoctoral fellow working jointly between the IBM Almaden Research Center and Stanford.

He began his pharmaceutical career at Merck in Rahway, NJ in 1997, moved to Transform Pharmaceuticals in 2002, and moved to Alkermes in 2008. At Merck, he was responsible for building a new pharmaceutical chemistry group to support basic research activities in Rahway, NJ. At Transform Pharmaceuticals/J&J he

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## CAREER DEVELOPMENT

Being an active participant in NESACS activities will enable you to network with major institutions and corporations in our area and can open up new career opportunities.

The NESACS Board of Publications, which is responsible for both the *Nucleus* newsletter and the NESACS website, is looking to increase its activities in this arena.

We would like to expand our capabilities for keeping our membership informed on what is happening in our field and how to adapt to changing times and new technologies.

You can help us do that. All we ask of you is a few hours a month and a smile.

Call or email to see what opportunities are available.

contact -- Vivian Walworth  
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Phone - 978-369-3735

Email [vwalworth@comcast.net](mailto:vwalworth@comcast.net)

# Abstract

## *Getting the most from salts and Cocrytals: formulating to maximize oral absorption*

The delivery, absorption and stability of pharmaceuticals is heavily dependent on their formulation. A rational approach to formulation requires an understanding of the physical and chemical properties of the drug itself, the proper selection of additional components, and the choice of preparative methods. Salt formation has been used with success, often on a trial-and-error basis.

A promising but so far little understood solution for delivery of poorly soluble or long-acting drugs involves the use of co-crystallization. This lecture will present new insights gained from investigation of the chemical, physical and spectroscopic characteris-

tics of candidate formulations, with the goal that the well-controlled formation of salts or co-crystallization may be exploited effectively in the design of new drugs

The delivery, absorption and stability of pharmaceuticals are heavily dependent on their physicochemical properties and on formulation. A rational approach to formulation begins with a detailed understanding of the properties of the drug itself.

Constructing the relationship between salts, cocrytals, or amorphous phases and the crystalline "free form" of the molecule is essential for overcoming solubility or dissolution rate limited absorption. Here, the goal is to choose forms and formulations that create and maintain supersaturated solutions of the drug. Crystalline salts have been used with success when the drug molecule can be easily ionized at physiological pH. However, the number of

*continued on page 12*

# Call for Nominations

## *The 2013 Theodore William Richards Award for Excellence in Teaching Secondary School Chemistry*

The Richards Award is the most prestigious award for high school chemistry teaching the Northeastern Section of the American Chemical Society offers in recognition of outstanding, innovative, and inspired teaching at the secondary level. It is intended to honor a teacher in the Northeastern Section who, through innovation and dedication, has inspired potential chemists, has communicated chemistry to non-chemists, or has influenced other teachers of chemistry.

The criteria for excellence correspond broadly to the effectiveness with which the teacher conveys chemistry, the innovative techniques used to help students comprehend chemical concepts, his/her interaction with students, both academic and extra-curricular,

and the influence a teacher has had on other teachers for promoting new approaches to teaching and learning.

The selected teacher will be officially honored and will receive both a \$1,500 prize and a Certificate of Recognition at the NESACS Education Night ceremony in May, 2013.

A complete description of the award, the nomination criteria, and nomination forms can be obtained from the NESACS website at: [http://www.nesacs.org/awards\\_richards.html](http://www.nesacs.org/awards_richards.html) Nominations are due no later than April 15, 2013 to the Richards Award Committee, attn: Steve Lantos, [steve\\_lantos@brookline.k12.ma.us](mailto:steve_lantos@brookline.k12.ma.us) (or via US Mail to: Steve Lantos, Science Department, Brookline High School, 115 Greenough St, Brookline MA 02445) ◇

Q. Exactly, how many awards and scholarships does NESACS sponsor?

A) One    b) Two    c) Many

[www.nesacs.org/awards](http://www.nesacs.org/awards)

# Robert Langer to Receive Major Awards

From the MIT News Office: <http://web.mit.edu/newsoffice/>

## 2013 Wolf Prize

David H. Koch Institute Professor Robert Langer of the Massachusetts Institute of Technology is among eight recipients worldwide of the 2013 Wolf Prize, the Israel-based Wolf Foundation announced.

The prestigious international prizes are awarded annually in five categories, each worth \$100,000. More than 30 Wolf Prize recipients have gone on to win the Nobel Prize.

Israeli President Shimon Peres will present the prizes in May at a special session hosted by the Knesset, the Israeli parliament.

## National Medal of Technology and Innovation

Robert Langer is among 23 eminent researchers nationwide who have been awarded the nation's highest honors, the National Medal for Science and the National Medal of Technology and Innovation for scientists, engineers and inventors, the White House announced.

Langer, the David H. Koch Institute Professor — who won a National Medal of Science in 2006 — will receive the National Medal of Technology and Innovation from President Obama at a ceremony to be held later this year.

For more detailed reporting see: [http://www.boston.com/yourcampus/news/mit/2013/01/mit\\_professor\\_to\\_be\\_honored\\_by\\_president\\_obama.html](http://www.boston.com/yourcampus/news/mit/2013/01/mit_professor_to_be_honored_by_president_obama.html) ◇

What exactly goes on at NESACS' monthly Board meetings?  
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# Announcement

## The Norris-Richards Undergraduate Summer Research Scholarships

The Northeastern Section of the American Chemical Society established the James Flack Norris and Theodore William Richards Undergraduate Summer Scholarships to honor the memories of Professors Norris and Richards by promoting research interactions between undergraduate students and faculty.

Research awards of \$3500 will be given for the Summer of 2013. The student stipend is \$3000 for a minimum commitment of ten weeks of full-time research work. The remaining \$500 of the award can be spent on supplies, travel, and other items relevant to the student project.

Institutions whose student/faculty team receives a Norris/Richards Undergraduate Summer Research Scholarship are expected to contribute toward the support of the faculty members and to waive any student fees for summer research. Academic credit

may be granted to the students at the discretion of the institutions.

Award winners are required to submit a report (~5-7 double-spaced pages including figures, tables, and bibliography) of their summer projects to the NESACS Education Committee by October 25, 2013 for publication in *The Nucleus*. They are also required to participate in the Northeast Student Chemistry Research Conference (NSCRC) in April 2014.

Applications will be accepted from student/faculty teams at colleges and universities within the Northeastern Section. The undergraduate student must be a chemistry, biochemistry, chemical engineering, or molecular biology major in good standing, and have completed at least two full years of college-level chemistry by Summer, 2013.

### Criteria for Selection:

- **scientific merit** - important factors include the originality of the project, the depth of the investigation, the significance of the scientific questions you pose, and the methods you propose to use.

- **feasibility** - evidence must be provided to demonstrate that the project can be completed by you in the time available and with the facilities at your disposal.

- **preparation** - your academic record, your ability to handle the project, and the background study you have made on your research problem will be taken into consideration.

- **commitment** - the depth of your commitment, and that of your department, faculty, and institution to independent research as a vital component of science education will be assessed.

Completed applications are to be submitted no later than **March 29, 2013**, to the Chair of the Selection Committee:

Professor Edwin Jahngen  
Department of Chemistry, Olney 520  
University of Massachusetts Lowell  
1 University Avenue  
Lowell, MA 01854

### Notification:

Applicants will be notified of the results by email on April 21, 2013, with written confirmation to follow. ◇

## Remenar Biography

*continued from page 5*

was responsible for improving the oral bioavailability of poorly soluble drug molecules and avoiding/overcoming physical and chemical stability problems in drug products. Through this work, he became interested in pharmaceutical co-crystals and in understanding where they fit into the spectrum of development options. At Alkermes, he has turned his attention to long-acting, injectable antipsychotics, through design of slowly dissolving crystalline prodrugs and through the understanding of phase behavior within polymeric microspheres. ◇

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# Summer Scholar Report

## Determination of the Reactivity of the Vibrational Ground State of Methane on Ni(111)

Patrick Kelleher\*, Cameron Hill\*, Yongli Huang\*\*, Nan Chen\*\*, Dr. Deno Del Sesto\*, Dr. Arthur Utz\*\*

\*Department of Chemistry, Stonehill College, Easton, MA, \*\*Department of Chemistry, Tufts University, Medford, MA

### Introduction:

A great deal of the field of chemistry revolves around the breaking and formation of bonds. The gas-surface dynamics of heterogeneous catalysis are of particular interest due to their pervasiveness in technology and chemical industry. Catalysts contribute towards roughly one third of the material GDP of the US economy<sup>1</sup> and also enable the Earth to sustain an additional 3.2 billion people via the ammonia fertilizer producing Haber-Bosch process.<sup>2</sup> Understanding exactly how the bonds of a gas molecule break in the presence of a metal catalyst would allow us to better predict and control these reactions in order to develop more efficient processes.

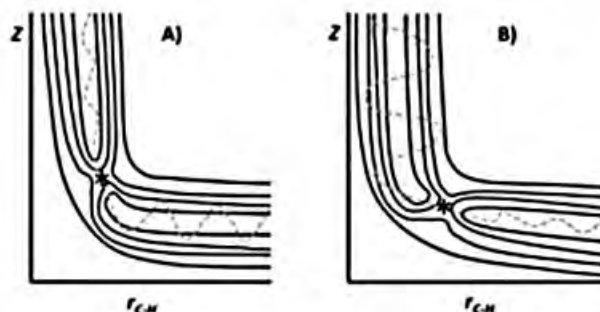
Our work focused on the reaction dynamics of methane on a Ni(111) surface. Methane is the main reagent in the steam reformation process, which is the source of 95% of hydrogen gas produced in the United States.<sup>3</sup> Methane is also of great interest from a theoretical standpoint. Its four different vibrational modes can be accessed with sufficiently long excited state lifetimes using infrared radiation, making it ideal for studying the effects of vibrational mode excitation on reactivity. Because methane is the simplest alkane, it is also the most basic gas in which C-H bond activation can be studied. Diatomic gases have only one fundamental vibrational mode and have been well studied. The vibrational modes of more complex polyatomic molecules are often indiscernible from one another and the mathematical tools needed to study them have not yet been developed.

### Background:

Statistical models have often been used to describe the scaling of reactivity with total energy. Recent work by the Utz group at Tufts University and others have pointed towards the existence of mode selective chemistry in which the reactivity does not solely depend on how much energy is put into a system but also how this energy is distributed.<sup>4</sup>

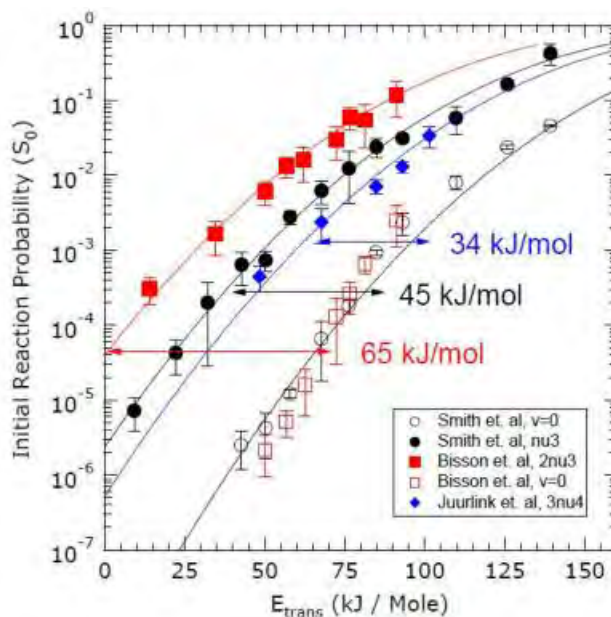
A prerequisite condition for mode selective chemistry occurring is that energy redistribution within individual molecules is sufficiently slower than the reaction time. Molecules that are selectively excited must remain excited long enough to react in order to influence reactivity. This condition being met makes mode selective chemistry possible, but does not ensure that it will occur. "Late" barrier reactions with geometrically "tight" transition states provide the best opportunity for vibrational energy to activate the reagent. A "late" transition state more closely resembles the products and requires a great deal of distortion of the reagent's equilibrium geometry. A geometrically "tight" transition state means the activation energy for the reaction increases sharply if the reaction complex varies from the ideal geometry. Vibrational modes that distort the molecule to resemble

the transition state will activate the reaction more so than other modes, producing mode selective behavior.



**Figure 1.** Two-dimensional Polanyi diagrams for methane adsorption.

Figure 1 shows two-dimensional Polanyi diagrams for the adsorption of methane on a surface. The contour lines show equal potential energy, and the saddle point is the energy of the transition state. The distance between carbon and hydrogen is denoted  $r$  and  $Z$  is the distance between hydrogen and the surface. Plot A represents the case where the reaction barrier, or saddle point, occurs in the translational coordinate (change in  $Z$ ) before the C-H bond stretches. This is an "early" barrier and translational energy would be expected to be the most effective at promoting reaction. Plot B represents the case where the reaction barrier occurs in the vibra-



**Figure 2.** Sticking curves for ground state and activated  $\text{CH}_4$  dissociation on Ni(111).<sup>6</sup>



## Summer Scholar

continued from page 8

tional coordinate (change in  $r$ ) where the C-H bond length is stretched. This is a “late” barrier and in this case vibrational energy would be expected to be the most effective at promoting reaction.

The Utz group<sup>4</sup> and Beck group<sup>5</sup> have performed a number of previous experiments to measure the reaction probability of methane on several surfaces. Differing reactivity for methane with the same total energy but different energetic configurations has been shown, identifying the vibrational modes that best promote transition state access for methane dissociation.

Figure 2 shows state-resolved reaction probabilities for methane dissociation on a Ni(111) surface at a surface temperature of 475 K. The filled in symbols denote reaction probabilities (black circles), (red squares), and (blue diamonds). Elevated nozzle temperatures are required to reach  $E_{\text{trans}}$  above 75 kJ/mol. Higher nozzle temperatures excite vibrational states in the molecules, which results in enhanced reactivity. This explains the deviation between the measured  $S_0^{\text{Laser Off}}$  (open symbols) and the solid curve approximating  $S_0^{v=0}$ . The thermal excitation of vibrational states at higher  $E_{\text{trans}}$  makes it difficult to interpret how each state contributes to the sticking probability. The difference in energy between the  $v=0$  curve and an excited vibrational state curve at a specific sticking probability is used to determine the vibrational efficacy. Determining an exact value for  $S_0^{v=0}$  rather than using a curve to approximate it would enable us to more accurately calculate the sticking probability contribution for each vibrational state using Equation 1.

$$S_0^{v=n} = \frac{S_0^{\text{laser on}} - S_0^{\text{laser off}}}{f_{\text{exc}}} + S_0^{v=0}$$

The goal of our research this summer was to experimentally determine a value for  $S_0^{v=0}$ . Sticking curves needed to be prepared for gas mixes with the same kinetic energy but different fractions of thermally excited molecules. This can be achieved by mixing methane with lighter or heavier gas to vary the energy of a molecular beam at a given temperature. The relationship between nozzle temperature and the fraction of excited molecules ( $f_{\text{exc}}$ ) follows a Boltzmann distribution. A second plot of sticking probability as a function of  $f_{\text{exc}}$  can then be made by taking vertical slices of the first plot. Each slice will have a specific kinetic energy and correspond to its own curve on the second plot.  $S_0^{v=0}$  is the sticking probability of a beam in which all molecules are in the ground state. By extrapolating to the y-axis ( $f_{\text{exc}}=0$ ) in the second plot, we can infer the ground state sticking probability at different kinetic energies. A final plot of the sticking probability as a function of kinetic energy at  $f_{\text{exc}}=0$  will give us reliable values for  $S_0^{v=0}$ .

## Experimental Procedure:

The Ni(111) crystal was cleaned each day by flashing above 1000K to bring impurities to the surface, followed by 5 minutes of argon ion sputtering to remove impurities, and finally annealing for 15 minutes at 1075K to recover a (111) ordered surface. Auger electron spectroscopy was used to confirm the surface was clean. Once cleanliness was verified, the Ni(111) was dosed with a molecular beam. The schematic of the molecular beam apparatus is shown in Figure 3. The IR laser is used in mode-selective experiments to excite vibrational modes of methane. Our experiment deals only with molecules in the ground state, so the laser was not used. The main chamber has a base pressure of approximately  $8 \times 10^{-11}$  torr and a pressure with the beam on of approximately  $1.7 \times 10^{-7}$  torr.<sup>7</sup> After each dose concluded all remaining gas was pumped from the chamber and the QMS was warmed up for analysis. The Ni(111) surface was exposed to a molecular oxygen beam created by the nozzle. Oxygen dissociates on the surface, reacting with adsorbed carbon to form CO which then desorbs. By monitoring the  $m/z=28$  signal, the amount of carbon on the surface can be determined. The total amount of carbon in each dose is dependent on the dose time, flux, and composition of the gas mix used.

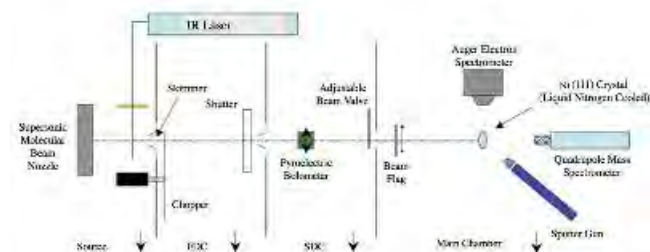


Figure 3. Molecular beam apparatus diagram.

## Results and Discussion:

Several data points were gathered for a nozzle temperature of 900K. A curve to model the data was created using IGOR Pro 5.03 software. The data follows a trend that was expected based on past studies. Sticking probability data needs to be gathered at several different nozzle temperatures ( $f_{\text{exc}}$ ) before further analysis can be carried out as discussed earlier.

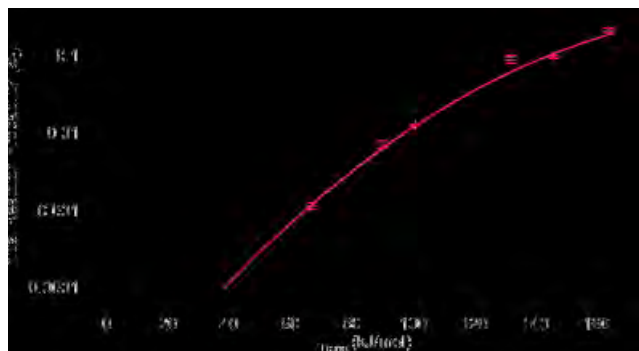


Figure 4. Sticking probabilities for  $T_N=900K$ .

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# January Meeting

A Report by Michael Filosa,  
Photos by Morton Z. Hoffman

If the January Meeting is a foreshadowing, we can expect a very interesting year of NESACS monthly meetings. Cathy Costello, the NESACS Chair-Elect for 2013 is the program chair for 2013. For the first seminar of the year, she asked her long-time professional colleague, Dr. Allen C. Steere of Harvard Medical School to speak at our first monthly meeting of the year about “*The Elucidation of Lyme Disease.*” The meeting was hosted in the 14<sup>th</sup> floor Hiebert Lounge at the Boston University School of Medicine of which Dr. Costello is a member of the faculty.



*Boston Skyline as seen from the Hiebert Lounge of the Boston University School of Medicine*

As *Nucleus* editor, I am involved in the publicizing of meetings and need information from the program chair for publication in the *Nucleus*. As I was waiting for biographical information, I decided to Google Dr. Steere and soon found that although his work is very well accepted by the scientific and medical establishment, there is a “Lyme disease counter culture” that is highly critical of the accepted treatment protocols for Lyme disease and question the fundamental science and the history of the origins of Lyme disease.

There are a large number of patients who believe they suffer from “Chronic Lyme Disease” and that they need to have continuous treatment of antibiotics to prevent the recurrence of symptoms. They claim the bacterium

can adopt a slow-growing form which hides undetected in the body and bursts forward in a relapse of symptoms (which can be extremely debilitating and life-threatening) once antibiotic treatment is stopped.

There are a number of physicians and politicians who support these patients and there have been laws passed in a number of states as a consequence of their advocacy to allow these treatments, which in general, are not supported by the scientific medical establishment or the insurance companies that have to pay for these treatments.

The scientific consensus is that a relatively long, single or double treatment of antibiotics kills the bacteria and stops the infection. The long-term effects suffered by some patients are a result of an auto-immune response to protein debris from the first infection or from a reinfection by another tick bite. Other explanations for the long-term symptoms exhibited by some patients are chronic fatigue syndrome, fibromyalgia, or psychiatric illnesses which are not a consequence of ongoing, resistant spirochete infection.

In addition to a history of the elucidation of Lyme disease, the recently demonstrated inflammatory properties of the protein debris from the infecting bacteria was a significant focus of Dr. Steere’s talk to about 50 NESACS members at our January Meeting.<sup>1</sup>

After reading a New York Times article from 2001 entitled “Stalking Dr. Steere over Lyme Disease,”<sup>2</sup> I was concerned that this meeting might be disrupted by the groups critical of Dr. Steere’s science. This elicited a substantial discussion before the meeting to make the section leadership aware of the potential for disruption.

I also, because of constraints posed by the publication deadline of the *Nucleus*, decided unilaterally to leave out the notice that “The Public is Invited” which has accompanied every meeting announcement published in the *Nucleus* for as long as I can remember.

The “Public is Invited” notification in our meeting notices became a subject of discussion at our board

meeting prior to the evening event. The NESACS Board voted that the “Public is Invited” to all of our monthly meetings and struggled to understand what the concern was for the upcoming talk by Dr. Steere. It was commented that science is often controversial.

In the week or so before the meeting, announcements of Dr. Steere’s upcoming talk were noticed by local (New Hampshire) Lyme disease activists and our secretary was emailed concerning the “controversial” nature of his talk and presented references counter to Dr. Steere’s work.<sup>3,4</sup>



*Dr. Catherine E. Costello introducing Dr. Allen C. Steere prior to his evening lecture on the “Elucidation of Lyme Disease.”*

After dinner, Dr. Steere was introduced by Dr. Costello and began his talk. It was a fascinating history about Lyme disease and its elucidation. He showed an idyllic river scene from Lyme, Connecticut and compared it to the Charles River in Dover, Sherborn and Medfield. He showed a fascinating map from the early days in which Lyme disease was discovered and its primary incidence in the Northeast and Midwest. The markers showing the occurrences were relatively scattered with the majority being in the Northeast. Near the end of the talk, he showed a truly frightening map<sup>5</sup> produced by the Center of Disease Control (CDC) which showed Lyme disease had spread exponentially since the late 1970’s and now blanketed most of the Northeast and upper Midwest and he predicted that the map would be filled in before too long along the Great Lakes including Illinois, Indiana and Ohio.

The cause of this spread was attributed to two factors. Deer were

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## January Meeting

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hunted to near extinction in the continental US as we entered the 20<sup>th</sup> century. As deer populations have thrived, Lyme disease has returned with a vengeance. In addition, a virulent form of the *Borrelia burgdorferi* bacterium is present in the Northeast which is particularly prone to induce the severe side-effects of the infection.<sup>6</sup>

The ancient nature of the disease was highlighted by a picture of the “ice-man,” Ötzi, the 5300 year-old mummy found frozen in a melting glacier in the Tyrolean Alps in 1991.<sup>7,8</sup> Ötzi was found through DNA analysis to have suffered from *Borrelia* infection.

As an example of a consequence of this inexorable spread, Medfield (the author’s home town) created a “Lyme Disease Advisory Committee” a few years ago and started a program at the end of 2011 to cull the deer population by bow hunting from its current 25 per square mile down to a safer 7-8 per square mile<sup>9</sup>.

The highlight of Dr. Steere’s talk was a slide summarizing his collaboration with Dr. Costello which identified, using tandem mass spectrometry, peptide factors from patients’ synovia produced by the infection. These factors were then synthesized and triggered an inflammatory reaction when reacted with the matching patient’s peripheral blood mononuclear cells. Even in a pre-inflammatory state in infected patients these factors were shown to have an enhanced inflammatory effect when compared to control cells from uninfected subjects.<sup>1</sup>

After Dr. Steere’s initial description of the identification of an unknown tick-borne disease in Lyme he then talked about the difficulty of identifying the pathogen. It took a number of years before reknowned researcher Willy Burgdorfer was able to successfully dissect *Ixodes* ticks and show convincing microscopic evidence of the *Borrelia burgdorferi* spirochete in the gut of the ticks. A scanning electron microscopic image of the spirochete obtained from one such dissection was another of the key sci-



Allen Steere (Harvard Medical School) presenting his talk, “The Elucidation of Lyme Disease.” entific advances presented by Dr. Steere.

While Dr. Steere was praising the skill and experience of Dr. Burgdorfer in identifying the Lyme disease pathogen through his unparalleled skill and experience, a spectator in the back suddenly interjected (paraphrasing), “But you don’t tell the whole story of how Burgdorfer in 1952 and 1956 did experiments to introduce *Borrelia* into ticks.” He was asked to identify himself. He gave his name, and said he was a filmmaker exposing the truth about Lyme disease.

As he was escorted out, he shouted out a brief verbal attack against Dr. Steere and the effect of Lyme disease

on his family.

The rest of the talk proceeded peacefully. Fortunately, unlike some of Dr. Steere’s presentations to Congress, our meeting was not packed with the opposition desiring to shout him down and contest his science. However, those in attendance did get a flavor of what Dr. Steere has faced the last 20 years for sincerely presenting his best science as he understands it.

It takes a pretty extreme and cynical view of science and government to believe that the tick-borne infections in Lyme, Connecticut are a product of biowarfare research gone wrong<sup>10</sup> or that the bulk of scientific presentations by the “establishment” are a vast conspiracy to cover up the “truth” about Lyme disease.

Regardless of the exact “truth” about Lyme infections, tick-borne infections by *Borrelia burgdorferi* spirochetes are a huge public health menace and tick-borne infections must be dealt with aggressively through education and reduction of tick populations by a variety of means.

Many thanks to Dr. Steere and Cathy Costello for this stimulating and

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## Summer Scholar

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### Future Work:

Due to time constraints and setbacks with the molecular beam apparatus during the summer we were only able to construct a curve for one temperature. Future work needs to be done to gather data for a range of other nozzle temperatures. Once sufficient data is collected it can be analyzed as discussed earlier and a curve for  $S_0^{v=0}$  as a function of kinetic energy constructed.

### Acknowledgments:

I would like to thank the Norris/Richards Undergraduate Summer Research Scholarship, my advisor, Dr. Deno Del Sesto (Stonehill College), our collaborator Dr. Arthur Utz, Stonehill SURE Scholar Cameron Hill, and the Utz Research Group at Tufts University including: Eric Dombrowski, Eric Peterson, Nan Chen, and Yongli Huang.

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## Student Summit

continued from page 4



Xin Su making his oral presentation, "When Aromaticity Met Resonance-Assisted Hydrogen Bonding (RAHB): Unusual para-Substituent Effects on the Intramolecular H-Bond in Hydration-Based switches"

we were still hopeful that progress towards our common goal could be made through practical suggestions, such as networking between the ACS and these stakeholders as well as making changes at the local level. All of these activities could sow the seeds for change in the right direction. I did leave the summit optimistic about some of these suggestions that we had made and also because of how our group came together. Even without the ACS-planned events during the trip, most of our group of international and domestic students would spend time with each other every night, going out to dinner and planning our own events. The last night was the best as we all went out to a couple of different night clubs in Raleigh. It might be the first and last time I will ever see more than ten dancing chemists in my life! We all made some great friends through this experience and knew that putting our best foot forward to discuss a complex problem was better than being apathetic toward the issue and the people around us.

We are especially grateful to the ACS and those most involved with us at the summit: Steve Meyers, Varsha Ramini, H. N. Cheng and Jodi Wesemann. ◇

<sup>i</sup> Gareis, E. *Journal of International and Intercultural Communication* 2012, 5, 309–312.

## Remenar Abstract

Continued from page 5

poorly soluble, difficult to ionize pharmaceutical candidates has increased dramatically in recent decades, leading to an explosion of research on cocrystals and stable amorphous materials.

This lecture will present new insights gained from investigating the interactions between drug molecules and formulation components during dissolution and will emphasize the importance of correlating changes in solubility with the physical form of the drug. ◇

## January Meeting

Continued from page 11

fascinating topic and to Boston University School of Medicine for hosting the first monthly meeting of 2013.

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# Meeting Notice

*American Chemical Society  
Central Massachusetts Section Meeting*

**Tuesday, March 5, 2013**

**Fitchburg State University**

Room 314, Hammond Bldg Tower, 160 Pearl St, Fitchburg, MA

**6:00 pm** Arrival, Refreshments

**7:00 pm** Lecture

J. Gregory Reid, Ph.D., *Mastering the 5000-L Rotavap and Other Challenges to Making Drugs on Industrial Scale*

## Directions

<http://www.fitchburgstate.edu/about-us/directions/>. Parking: North Street Lots 1 and 2 - #5 & 6 on Campus Map.

(<http://www.fitchburgstate.edu/uploads/files/Directions/ParkingLotMap.pdf>).

Hammond Building is the adjacent brick and glass building with the glass tower in the center. Room 314 is on 3rd floor. Please RSVP Host/Contact: Dr. Mel Govindan – [mgovindan@fitchburgstate.edu](mailto:mgovindan@fitchburgstate.edu); Cell: 978-660-8831.

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**Petition Candidates:** “Any group comprising 2 per cent or more of the North-eastern Section (136 members) may nominate candidates...” See NESACS website for details. ◇

## Abstract

After spending years figuring out processes to make grams of complex molecules in a lab, I began to wonder how they are made on very large scale in industry. This continued as I started work as a process chemist at a major drug company. One of the challenges - understanding and controlling reactions - was still very important, but a lot of additional challenges were added. Process safety, purifications, raw material constraints (due to both cost and safety), productivity, reactor limitations, reuse/recycle of waste streams, etc. became important considerations. Many of these challenges will be highlighted with entertaining real-life examples of process R&D, including a comparison with how this work is done in India. Students are particularly encouraged to attend. ◇

## Biography

J. Gregory Reid decided he wanted to invent beautiful processes to make drugs while he was studying chemistry at the University of Michigan. After earning a PhD with Ed Vedejs at the University of Wisconsin and doing postdoctoral research with E. J. Corey at Harvard, he accepted a position as a Scientist in Chemical Process R&D at Upjohn. Since then his career has included 13 years at Big Pharma doing process R&D, 2 years starting and managing a successful custom synthesis company, 8 years at different Contract Research Organizations (CRO) in the US, 2 years at a CRO in India, and 2 years as a visiting professor at Union College in Schenectady. He is currently a chemistry consultant working out of his home in Groton, MA. ◇

## January Meeting

*Continued from page 12*

[iceman-s-dna-reveals-health-risks-and-relations-1.10130](#)

<sup>9</sup> James O'Brien, Boston.com, October 11, 2011. <http://www.boston.com/news/local/>

[articles/2011/10/16/deer\\_hunt\\_in\\_med-field\\_takes\\_aim\\_at\\_lyme\\_disease/](#)

<sup>10</sup> Michael Braverman, Germs Gone Wild: The Horrific Secrets of Plum Island <http://www.trutv.com/conspiracy/government-lies/plum-island/lyme-disease.html> ◇

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pages for travel directions and updates.

These include:

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### Mar 04

Prof. Yi Lu (Illinois State Univ.)

“Rational Design of Metalloproteins as Biocatalysts for Sustainable Energy: Exploring Roles of Non-covalent Interactions in Conferring and fine-tuning Enzymatic Activities”  
Brandeis, Gerstenzang 121  
4:00 p.m.

Prof. Todd Lowary (Univ. of Alberta)

“Amphiphilic Mycobacterial Glycans: Synthesis, Biosynthesis and Lipid-binding Properties”  
Northeastern Univ. 129 Hurtig Hall  
12:00 noon

Prof. David Speigel (Yale University)

Harvard, Pfizer Lecture Hall, TBA,  
4:15pm

### Mar 05

Zachary Kean (Duke University)  
UNH, Room N104 (formerly L103)  
11:10 am

Prof. Todd Lowary (Univ. of Alberta)

“Furanoside biosynthesis in mycobacteria and campylobacters”  
Tufts, Pearson Chemistry Building, Room P-106  
4:30 pm

### Mar 06

Prof. Clay Bennett (Tufts)  
U. Mass. Dartmouth, SENG, Room 115  
4:00 PM

### Mar 11

Prof. Jack Taunton (U. C. San Francisco)  
Harvard, Pfizer Lecture Hall,  
4:15pm

Prof. David Jenkins (University of Tenn.)  
Brandeis, Gerstenzang 121 4:00 p.m

Prof. Erin E. Carlson (Indiana Univ.)

“Chemical Probes to Explore and Inhibit Bacterial Growth and Pathogenesis”  
MIT, 56-114  
4:00 pm

### Mar 12

Prof. David Anderson (University of Wyoming)  
“Cold Chemistry in Parahydrogen Quantum Solids: What Arrhenius Didn’t Tell You”  
MIT, 6-120  
4:30 pm

Prof. Kenichi Kuroda (University of Michigan)  
“Designing antimicrobial polymers as synthetic mimics of host-defense peptides”

Tufts, Pearson Chemistry Building, Room P-106  
4:30 pm

### Mar 13

Prof. David Jenkins (Univ. of Tennessee)  
MIT, 6-120  
4:15 pm

Prof. James Chambers (U. Mass.-Amherst)  
WPI, Gateway Park, Rm. 1002  
12:00 Noon

### Mar 18

Prof. Seth Herzon (Yale)  
“Target-Driven Total Synthesis”  
Brandeis, Gerstenzang 121 4:00 p.m.

Prof. Kevin Weeks, University of North Carolina, Chapel Hill  
MIT, 56-114 4:00 pm

### Mar 19

Prof. Eli Zysman-Colman (Université de Sherbrooke, Canada)  
“Illuminating Iridium: From Visual Displays to Solar Cells”  
Boston College, Merkert 130  
4:00 PM

Prof. Liviu Mirica (Washington Univ.)  
Harvard, Pfizer Lecture Hall, 4:15pm

### Mar 20

Prof. Liviu Mirica (Washington Univ.)  
MIT, 6-120  
4:15pm

Prof. Chris Douglas (Univ. of Minnesota)  
“Catalysis based on the insertion of transition metals adjacent to carbonyls: carbonylation, oxyacylation and hydroacylation of alkenes”  
Northeastern Univ. 129 Hurtig Hall  
12:00 noon

Boston College University Lecture Series in Chemistry  
Prof. Dennis A. Dougherty (California Institute of Technology)  
“Chemistry on the Brain: Understanding the Nicotine Receptor”  
Boston College, Merkert 127  
4:00 - 5:00 PM

### Mar 20 -21

Iddles Lecture Series

Prof. Mark A. Ratner (Northwestern University)  
3/20 “Sustainability and Energy - The Story of our Time”  
3/21 TBA  
UNH, Room N104 (formerly L1030)  
11:10 am

### Mar 21

Bristol-Myers Squibb Lectures in Organic Chemistry

Prof. Tobias Ritter, Harvard  
Jeffrey Robl, Bristol-Myers Squibb  
MIT, 6-120  
4:00 pm

Boston College University Lecture Series in Chemistry

Prof. Dennis A. Dougherty (California Institute of Technology)  
“The Cation- $\pi$  Interaction: A New View of Benzene, Phe, Tyr, and Trp”  
Boston College, Merkert 127 4:00 pm

### Mar 22

Boston College University Lecture Series in Chemistry

Prof. Dennis A. Dougherty (California Institute of Technology)  
“Chemical-Scale Studies of Neuroreceptors and Ion Channels: What Have We Learned?”  
Boston College, Merkert 127 2:30 pm

### Mar 25

Prof. Andrew Phillips (Yale)  
Harvard, Pfizer Lecture Hall, 4:15pm

Prof. William M. Clemons (California Institute of Technology)  
MIT, 56-114 4:00 pm

### Mar 26

TISHLER AWARD LECTURE

Prof. Roderick MacKinnon (Rockefeller University)  
“The Remarkable Diversity of K<sup>+</sup> Channels”  
Tufts, Pearson Chemistry Building, Room P-106  
4:30 pm

Prof. Kay Brummond (University of Pittsburgh)  
UNH, Room N104 (formerly L1030)  
11:10 am

### Mar 27

Prof. Jens Nørskov (School of Engineering, Stanford Univ.)  
Northeastern Univ., 129 Hurtig Hall  
12:00 noon

Prof. Timothy Warren (Georgetown Univ.)  
Harvard, Pfizer Lecture Hall 4:15pm

### Mar 28

Prof. Haekjip Ha (University of Illinois)  
Harvard, Pfizer Lecture Hall 4:15pm

Notices for The Nucleus  
Calendar of Seminars should be sent to:

Sheila E Rodman, email:  
serodman(at)hotmail.com